

Stripe phase ordering as quantum interference phenomenon.

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Abstract

A quantum interference mechanism of the stripe phase instability in quasi one-dimensional (1D) repulsive electron system is proposed. The leading spin-charge coupling term in Landau functional is derived microscopically. It is shown that away from half filling, periodic lattice potential causes cooperative condensation of the spin and charge superlattices, which constitute a 1D analogue of the experimentally observed quasi 2D structures in lanthanum cuprates and nickelates. Renormalization group analysis qualitatively supports the Hartree-Fock picture.

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Stripe phases recently observed in doped antiferromagnets [1] attract attention to the problem of multi-mode instabilities in the interacting electron systems [2]-[4]. Spin and charge modulations found in the doped layered transition metal oxides possess locked mutual phase and doping dependent periods, incommensurate with the period of the underlying crystal lattice. Period of the spin modulation is twice the period of the charge modulation. An onset of this picture in CuO_2 and NiO_2 atomic planes is detected by neutron scattering experiments [1] which, below some temperature, reveal two systems of intense superlattice peaks. Locations of the spin and charge peaks in the two-dimensional square Brillouin zone are: $(1/2 \pm \epsilon, 1/2)$ for spin and $(\pm 2\epsilon, 0)$ for charge; as well as at $\pi/2$ rotated positions: $(1/2, 1/2 \pm \epsilon)$ and $(0, \pm 2\epsilon)$. Here units of $2\pi/a$ are used, and a is the lattice period. For small enough doping concentration, x_d , a relation holds: $\epsilon \sim x_d$, and at greater x_d 's a shoulder develops. Commensurate antiferromagnetic order at half filling (i.e. at $x_d = 0$) is characterized with the wave vector $\vec{Q}_{AF} = (1/2, 1/2)$. Existing theoretical works on the stripe phase instability either find variationally the ground state of the microscopic models [2,3], or use phenomenological Landau-Ginzburg functional constructed by symmetry considerations [4].

In this Letter we propose a quantum interference mechanism of the stripe phase instability in (quasi) one-dimensional (1D) electron system, brought about by the periodic lattice potential. A microscopic derivation is presented of the main spin-charge coupling term in the Landau functional, which was phenomenologically introduced in [4]. A model considered below was already investigated in the Hartree-Fock approximation [3], but proposed here mechanism of the stripe phase ordering was not discussed. Neither was it discussed in the previous studies of the 1D electron systems within one-loop renormalization group approach [5] ("parquet" formalism), which is considered in the last part of this Letter.

We start from the Hartree-Fock approximation. The Hubbard Hamiltonian with the hopping integral t and on-site repulsion U (> 0) may be written in the form:

$$H = t \sum_{\langle i,j \rangle \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i \left(\frac{1}{4} \hat{n}_i^2 - (\hat{S}_i^z)^2 \right) \quad (1)$$

Here an identity: $\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = \frac{1}{4}\hat{n}_i^2 - (\hat{S}_i^z)^2$ was used. Operators $\hat{n} \equiv \hat{n}_\uparrow + \hat{n}_\downarrow$ and \hat{S}^z are fermionic density and spin (z-component) operators respectively, and σ is spin index. Hamiltonian (1) has convenient form for the Hartree-Fock decoupling in the presence of two, i.e. spin and charge, order parameters. At half filling, i.e. at one electron per site, the system orders antiferromagnetically [6,7]: $S_i^z = (m_o/2) \cos(\vec{Q}_{AF}\vec{r}_i)$. Away from half filling, mean-field approximation [8] predicts a spin density wave (SDW) instability in the continuous quasi 1D system: $S^z(x) = (m_o/2) \cos(Q_-x - \phi)$, with the incommensurate wave vector $Q_- = 2k_F$. In the weak coupling limit, $U \ll t$, the SDW instability is brought about by the existence of the nested parts of the Fermi surface separated by momentum $2k_F$. The difference $Q_{AF} - Q_- \equiv 1/2 - 2k_F = \epsilon$ is expressed via the hole (electron) doping concentration $x_d > 0$ ($x_d < 0$) as: $\epsilon = x_d/2$. Effect of the periodic lattice potential away from half filling has been so far neglected, both in the mean-field and in the "parquet" approaches [8,5].

Consider an incommensurate SDW expression, $S^z(x_i) = (m_o/2) \cos(Q_-x_i - \phi)$, on a chain. Here x_i is the "site coordinate" along the chain, and ϕ is a phase shift. Allowing for the periodicity of the lattice sites, $x_i = N_i a$; $N_i = 0, \pm 1, \pm 2, \dots$, we may rewrite the cosine in the SDW expression in the equivalent form (x_i is taken in units of a): $\cos(Q_-x_i - \phi) = (1/2)(\cos(Q_-x_i - \phi) + \cos(Q_+x_i + \phi)) = \cos(x_i/2) \cos(\epsilon x_i + \phi)$; where $Q_+ = 2\pi/a - Q_-$, i.e. $1/2 + \epsilon$ in our dimensionless units. These simple relations demonstrate significant physical fact that an incommensurate SDW on the lattice can be decomposed into two umklapp related SDW's, which could be called "direct" ($Q_- = 2k_F$) and "shadow" ($Q_+ = 2\pi/a - 2k_F$) waves [9]. It is wellknown [10] that formation of SDW with wave vector Q may be regarded as Bose-condensation of electron-hole pairs $c_{k,\sigma} c_{k+Q,\sigma}^\dagger |O\rangle$ with momentum Q ($|O\rangle$ is unperturbed vacuum state of the Fermi-system). In our case this means formation of the *two* electron-hole condensates, with wave vectors Q_\pm , corresponding to "direct" and "shadow" SDW's. Then, scattering of electrons (holes) by some "extra" periodic potential with "matching" wave vector $Q_+ - Q_- \equiv 2\epsilon$ would cause quantum interference between the wave functions of the Q_\pm condensates. At some value of the relative phase shift the interference may become constructive, causing enhancement of the gap in the fermionic quasi-particle spectrum of the quasi 1D electrons and related decrease of their total (free) energy. Here we consider a charge density wave (CDW): $\rho(x) = \rho_o \cos(Q_+ - Q_-)x$, as an option for the "matching" extra potential. Depending on the balance between the gain of energy and the "cost" of the CDW formation, a condensation of the coupled SDW-CDW phase takes place as a first/second order phase transition. This state, consisting of "direct" and "shadow" SDW's and "matching" CDW, with locked relative phase shift ϕ , is right a weak coupling analogue of the stripe phase order considered in the literature [1]- [4].

In the presence of the SDW and CDW condensates, i.e. densities $m(x)$ and $\rho(x)$ introduced above, the single-particle eigenstates of the Hamiltonian Eq.(1) in the Hartree-Fock approximation can be determined from the Bogoliubov-de Gennes equations derived in [3]:

$$\mp i2t \frac{\partial u_{\pm}}{\partial x} + \frac{U}{2} \rho(x) u_{\pm} - \frac{U}{2} \tilde{m}(x) u_{\mp} = E u_{\pm} \quad (2)$$

Here left- and right-movers representation is used for the quasi-particle wave function: $\psi_{\sigma}(x) = u_{+}(x) \exp(ix/4) + \sigma u_{-}(x) \exp(-ix/4)$, and coordinate x is expressed in units of the chain period, a . The spin density is: $m(x_i)/2 = (m_o/2) \cos(Q_- x_i - \phi) = \tilde{m}(x_i) \cos(x_i/2)$, so that: $\tilde{m}(x) \equiv (m_o/2) \cos(\epsilon x + \phi)$. Thus, only slowly varying functions $u_{\pm}(x)$, $\tilde{m}(x)$ and $\rho(x)$ are involved in Eq.(2). Now, instead of dropping CDW term, $\rho(x)u_{\pm}$, from Eq.(2) [3], we shall explicitly allow for it by writing wave functions $u_{\pm}(x)$ in the Bloch wave basis of the periodic CDW potential:

$u_{\pm}(x) \equiv c_{\pm}^k \exp(ikx \mp iU/(2v) \int^x \rho(x') dx') \approx c_{\pm}^k e^{ikx} \{J_0(z) \mp J_1(z) (e^{i2\epsilon x} - e^{-i2\epsilon x})\}$; where $v = 2t$ is the Fermi velocity of electrons, and $z = U\rho_o/(2v\epsilon)$. Here J_n is the Bessel function of the integer order n , and the terms of higher orders than $n = 1$ are neglected, provided that $U\rho_o/(2v\epsilon) \leq 1$. After substitution of $u_{\pm}(x)$ in the above representation into Eq. (2) one finds an algebraic system of linear homogeneous equations for the coefficients c_{\pm}^k . Solving corresponding determinant equation one finds the single-particle spectrum:

$$E_k = -\frac{v\epsilon}{2} \pm \sqrt{\left(k + \frac{\epsilon}{2}\right)^2 v^2 + \Delta^2}; \quad (3)$$

$$\Delta \equiv \frac{Um_o}{4} f\left(\frac{U\rho_o}{2v\epsilon}\right) \\ f(z)^2 \equiv J_0^2(z) - 2\cos(2\phi)J_0(z)J_1(z) + J_1^2(z) \quad (4)$$

In the "electron doping" case the sign in front of ϵ in Eq.(3) and of $\cos 2\phi$ in Eq. (4) should be changed. The physical implication of Eqs. (3), (4) is remarkable. Namely, in the presence of the CDW the effective coupling constant $Uf(z)$, responsible for the SDW condensation, is enhanced with respect to bare coupling U , provided $f(z) > 1$. The latter condition fixes $\cos(2\phi)$. The form of Eq.(4) manifests quantum interference between scattering amplitudes of electron in the combined periodic potentials of Q_{\pm} -SDW and $(Q_+ - Q_-)$ CDW. A simple form of solution (3) is valid in the weak coupling limit, $U \ll t$, not too close to half filling, i.e. when $x_d \gg \Delta/t$. Also, despite the gap in the spectrum (3), the system may remain conductive due to sliding of the incommensurate density waves along the lattice.

Free energy of the system (per unit of length), Ω , at finite temperature $T(\equiv \beta^{-1})$, follows from Eq.(3) and the Hartree-Fock form [3] of the Hamiltonian (1):

$$\Omega = (U/8)(m_o^2/2 + \rho_o^2) - (4T/\pi v) \int_0^{E_b} \ln [2 \cosh(\beta E(\xi)/2)] d\xi \quad (5)$$

where $E(\xi) = \sqrt{\xi^2 + \Delta^2}$, and $E_b(\sim t)$ is the upper cutoff of the electron energy. Due to interference term $-2\cos(2\phi)J_1(U\rho_o/2v\epsilon)J_0$ in Eq.(4), the lowest order expansion of Ω , Eq.(5), in powers of the CDW amplitude (at small m_o) yields linear in ρ_o term: $\delta\Omega \sim -m_o^2\rho_o U^2/(tx_d)$. This term reveals possible microscopic origin of the corresponding spin-charge coupling term in the phenomenological Landau-Ginzburg functional considered in [4].

Here we merely list the main results following from Eq.(5).

i) Coming from the high temperature limit, $\Delta = 0$, the stripe phase condenses first with $\cos(2\phi) = -1$ or $\cos(2\phi) = 1$ depending on the sign of x_d . Thus, the spin density behaves as: $\langle 2S^z(x) \rangle = -m_o \cos(x/2) \sin(\epsilon x)$ in the case $x_d > 0$, and as : $\langle 2S^z(x) \rangle = m_o \cos(x/2) \cos(\epsilon x)$ in the $x_d < 0$ case. Simultaneously, electron charge density is the same in both cases: $-\rho_o \cos(2\epsilon x)$. Hence, the nodes of the spin density coincide with the minima (maxima) of the charge density $\rho(x)$ in the case of the hole (electron) doping. This topology is in accord with the stripe phase topology considered in the strong coupling limit [2]- [4].

ii) When doping concentration x_d decreases below $x_o \sim \sqrt{t/U} \exp(-2\pi t/U)$ the system enters strong coupling regime, see Figs. 1,2. This transition is governed by dimensionless parameter $:U\rho_o/(2\pi t x_d)$. At $U\rho_o/(2\pi t x_d) \geq 1$ higher order Bessel functions contribute to the wave function $u_{\pm}(x)$ and a few-harmonic approximation, resulted in Eqs.(3), (5), fails. This indicates a solitonic, rather than SDW-CDW structure of the stripe phase in the lowest doping limit, $x_d \rightarrow 0$, in a qualitative accord with the previous proposals [2,3]. Stripe phase condensation temperature, T_c , monotonically decreases from the *highest* value $T_m = 2(\gamma/\pi)t \exp(-2\pi t/(U f_m^2))$ at small doping concentrations, $|x_d| < x_o$, to the *lowest* value $T_{SDW} = 2(\gamma/\pi)t \exp(-2\pi t/U)$ at $|x_d| \gg x_o$. Here $\gamma = 1.78$, and $f_m \equiv f(z_m) \approx 1.2$ is the maximum value of the function $f(z)$ in Eq.(4), reached at $z = z_m \approx 0.83$. The drop of T_c is accompanied by a substantial decrease of the SDW and CDW amplitudes at zero temperature, see Fig. 1:

$m_o = 8t/U \exp(-2\pi t/U)$, at $x_d \gg x_o$; and $m_o = 8t/(U f_m) \exp(-2\pi t/(U f_m^2))$, at $x_d \ll x_o$.

Simultaneously, the character of the phase transition changes at x_o from the *first order* ($x_d < x_o$) to the *second order*, Fig. 2. The jumps of the CDW and SDW amplitudes at the first order transition temperature are: $m_o^2 \approx x_d z_m T_m \sqrt{2\pi t U} / (U f_m)^2$ and $\rho_o \approx 2\pi x_d z_m t / U$. The latter estimate for ρ_o results in the following value of the "small parameter": $U\rho_o/(2\pi t x_d) \approx 0.83 < 1$. Hence, our results in the region $x_d < x_o$, based on the neglect of the higher order SDW/CDW harmonics, might be considered as qualitative rather than quantitative.

iii) In the second order phase transition regime, $|x_d| \gg x_o$, the order parameters close to T_c behave as: $\rho_o \approx 3\tau T_{SDW}^2 / (x_d t U)$, and $m_o \approx 12\sqrt{\tau} T_{SDW} / U$; in qualitative accord with [4] (here $\tau \equiv 1 - T/T_{SDW}$). In the classification of [4] the phase transitions described in ii), iii) above belong to the "spin-charge coupling driven" and "spin driven" kinds.

Important issue for the (quasi) 1D systems is the influence of fluctuations. We study it within a single-loop renormalization group (RG) scheme, so-called "parquet" approximation [5], which we adjust for the case of the two order parameters (SDW/CDW) coupled already on the mean-field level. Conventionally, "parquet" - RG equations describe behavior of the two-electron scattering vertices $\gamma_1(\xi)$, $\gamma_2(\xi)$, and $\gamma_3(\xi)$, accounting for back-, forward-, and umklapp scattering of electrons respectively close to the Fermi "surface" points: $\pm k_F$. The RG variable, ξ , is the logarithm of the infrared cutoff of the energy/momentum transfer. It is involved in the (logarithmically) diverging corrections to the vertices, which are initially defined in the Born approximation: $g_i \equiv \gamma_i(\xi = 0)$. Within "parquet" approach only corrections

of the highest power in ξ are retained in each order of the perturbation expansion in each γ_i and then summed to an infinite order. An instability of the electron system is manifested by divergences of the (initially finite) vertices $\gamma_i(\xi)$ at some finite value ξ_o . In the case of the Hubbard Hamiltonian (1) at half filling: $g_i = U/(4\pi t)$, $i = 1, 2, 3$, in the dimensionless units. Away from half filling the umklapp condition: $p_1 + p_2 = p_3 + p_4 \pm 2\pi/a$, can not be fulfilled when all the quasi-momenta of electrons (before and after scattering) are close to the Fermi surface. In conventional "parquet" theory [5] an instability does not occur in repulsive 1D system without umklapp, i.e. when $g_1, g_2 > 0$, $g_3 = 0$. In the (hole) doped case the deficiency of momentum transfer: $2\pi/a - 4k_F \equiv 2\epsilon = x_d \neq 0$, provides a "natural" momentum cutoff, such that at $\xi > \xi_d \equiv \ln(1/x_d)$ the growth of $|\gamma_i(\xi)|$ terminates. Hence, in the standard approach [5], an instability at ξ_o would be only possible if $\xi_o < \xi_d$, i.e. in the low doping region: $x_d < x_1 \equiv \exp(-\xi_o)$. In this region commensurate SDW is indistinguishable from incommensurate one within a logarithmic accuracy of "parquet" with respect to the infrared momentum cutoff. Using estimate [5]: $\xi_o \sim 2\pi t/U$, we find: $x_1 = \exp(-2\pi t/U)$, which is inside our mean-field "strong coupling" region: $x_d < x_1 < x_o$. In order to probe the system for a stripe phase instability in the region: $x_d > x_1$, where incommensurability is well resolved, we modify "parquet" treatment by adding fictitious "stripe phase" vertices $\tilde{\gamma}_i(\xi)$ with infinitesimal "starting" values $\tilde{\gamma}_i(\xi_d)$ at $\xi_d < \xi_o$. The vertices $\tilde{\gamma}_{1,2}(\xi)$ describe "umklapp" scattering with the wave vector $2\epsilon = x_d$, brought by the CDW component of the stripe phase; while $\tilde{\gamma}_3(\xi)$ is due to combined lattice-CDW umklapp: $2\pi/a - 2\epsilon$. Thus, "enriched" RG-"parquet" equations in the interval $\xi_d < \xi < \infty$ become:

$$\begin{aligned}\dot{\gamma}_3(\xi) &= -2\tilde{\gamma}_3(\xi)\tilde{\gamma}_4(\xi); \quad \dot{\tilde{\gamma}}_4(\xi) = -4Re(\gamma_3(\xi)\tilde{\gamma}_3^*(\xi)) \\ \dot{\gamma}_4(\xi) &= -2\tilde{\gamma}_3(\xi)\tilde{\gamma}_3^*(\xi); \quad \dot{\tilde{\gamma}}_3(\xi) = -2\tilde{\gamma}_3(\xi)\gamma_4(\xi)\end{aligned}\tag{6}$$

where $\gamma_4(\xi) = \gamma_1(\xi) - 2\gamma_2(\xi)$, and same relation is valid between $\tilde{\gamma}_4$ and $\tilde{\gamma}_{1,2}$ [11]. Diverging solutions of Eqs.(6) for two concentrations $x_i > x_1$ are shown in Fig. 3. Analytical solution in the interval $\xi > \xi_d$ is: $\gamma_3(\xi) = B \cosh(C \ln |\tanh D(\xi - \tilde{\xi}_o)| + \phi_o)$; $\tilde{\gamma}_4(\xi) = \pm \sqrt{2(\gamma_3^2 - B^2)}$; $\gamma_4(\xi) = (D/2) \coth 2D(\xi - \tilde{\xi}_o)$; $\tilde{\gamma}_3(\xi) = DC/(\sqrt{2} \sinh 2D(\xi - \tilde{\xi}_o))$, where $\tilde{\xi}_o \sim \xi_o + 0.5(\xi_o - \xi_d) \ln(2/|\tilde{\gamma}_i(\xi_d)|)$, and all the constants are determined from the boundary conditions for γ_i and $\tilde{\gamma}_i$ at $\xi = 0$ and $\xi \approx \xi_d$ respectively.

The divergence of the probe vertices $\tilde{\gamma}_i(\xi)$ signals [5] in favour of spontaneous incommensurate (stripe) ordering in the ground state of the system away from half filling. Though, neither mean-field, nor "parquet" approximation gives decisive answer about the long-range order and/or gap in the quasi-particle spectrum of 1D system [5].

In conclusion, a quantum interference mechanism of the stripe phase ordering in repulsive (quasi) 1D electron system is proposed. Preliminary 1D renormalization group ("parquet") analysis does not contradict the mean-field construction. Substantial enhancement of the stripe ordering temperature due to interference between charge and spin order amplitudes is found. Analysis of analogous possibility for the superconducting order parameter is now in progress.

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I. FIGURES

Fig.1. SDW (m_o) and CDW (ρ_o) stripe phase order parameters, as functions of doping concentration x_d at zero temperature, calculated using Eq.(5). Inset: normalized stripe phase transition temperature T_c as function of doping. $4t/U=3.2$.

Fig.2. Calculated temperature dependences of the stripe phase order parameters, m_o (curves labeled with "m") and ρ_o (curves not labeled) for the different doping concentrations x . Each pair of lines of the same type (e.g. solid, dashed, etc.) show m_o and ρ_o for each particular value of doping concentration x . $4t/U=3.2$.

Fig.3. Solid lines: numerical solutions of the Eqs.(6) for the vertices $\gamma_{3,4}$ (curves 3 and 4 respectively) and $\tilde{\gamma}_{3,4}$ (curves 3' and 4' respectively), for values of $\xi_d = \xi_{1,2} < \xi_o$. Dashed lines: same as above, but for $\xi_d > \xi_o$. Starting values: $g_{1,2,3} = -g_4 = 0.1$; $\tilde{\gamma}_3(\xi_i) = -\tilde{\gamma}_4(\xi_i) = 0.01$.





